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On the Extremal Mostar Indices of Hexagonal Chains

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Abstract

For a given graph G, the Mostar index $Mo(G)$ is a bond-additive topological index as a measure of peripherality in G. Došlić et al. (2018) posed an open problem: Find extremal benzenoid chains, catacondensed benzenoids and general benzenoid graphs with respect to the Mostar index [7]. In this paper, we partially solve above problem, i.e., sharp upper and lower bounds on the Mostar indices among hexagonal chains with a given number of hexagons are determined, respectively. All the corresponding extremal hexagonal chains are characterized.

1. Introduction

In this paper, all the graphs we considered are connected, simple and undirected. All the notations and terminologies not defined here we refer the reader to Bondy and Murty [2].

Let $G = (V_G, E_G)$ be a graph with the vertex set V_G and the edge set E_G. For a vertex $v \in V_G$, we denote the degree of v by $d_G(v)$ (or d_v if no ambiguity is possible). If $d_G(v) = 1$, then v is called a *pendant vertex* of G. For a set U, denote by $|U|$ its cardinality. For a vertex subset S of V_G, denote by $G[S]$ the subgraph of G induced by

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S. As usual, P_n denotes the path with n vertices. The *distance*, $d_G(u,v)$ (or $d(u,v)$ for short) between two vertices u,v of G is the length of a shortest u-v path in G.

For each edge $e = uv \in E_G$, let

$$\begin{aligned} N_G^u(e) &= \{x \in V(G) | d(x,u) < d(x,v)\}, \\ N_G^v(e) &= \{x \in V(G) | d(x,u) > d(x,v)\}, \\ N_G^0(e) &= \{x \in V(G) | d(x,u) = d(x,v)\}. \end{aligned}$$

and let $n_G^u(e) = |N_G^u(e)|$, $n_G^v(e) = |N_G^v(e)|$, $n_G^0(e) = |N_G^0(e)|$. For convenience, put $n_u := n_G^u(e)$, $n_v := n_G^v(e)$ and $n_0 := n_G^0(e)$, respectively, if no ambiguity is possible. Clearly, one has $V_G = N_G^u(e) \cup N_G^v(e) \cup N_G^0(e)$. If in addition G is bipartite, then we get $N_G^0(e) = \emptyset$ and $n_0 = 0$. Otherwise, if there exists $x \in N_G^0(e)$, then a shortest u-x path, a shortest v-x path and the edge e implies an odd cycle, which is a contradiction with G is bipartite.

Specially, a graph G is *distance-balanced* if $n_u = n_v$ for each edge $uv \in E_G$. Jerebic, Klavžar and Rall [10] investigated the basic properties of distance-balanced graphs. The symmetry conditions were studied in [12]. For more details of distance-balanced graphs, one may be referred to [1, 9, 13] and the references cited therein. But there exists many graphs which are not distance-balanced. Hence, how far is a graph from being distance-balanced has received much attention. In 2018, Došlić et al. [7] proposed a new structural invariant of graphs, called *the Mostar index*, which is defined as

$$Mo(G) = \sum_{e=uv \in E(G)} \phi_G(e), \tag{1.1}$$

where

$$\phi_G(e) = |n_u - n_v| \tag{1.2}$$

is called the *contribution* of the edge $e\,(= uv)$ for $Mo(G)$.

Clearly, a graph G is distance-balanced if and only if $Mo(G) = 0$. The Mostar index produces a global measure of peripherality of G by calculating the sum of peripherality contributions over all edges in G. Very recently, studying the extremal values of the Mostar index among graphs have attracted researchers' attention. In 2018, Došlić et al. [7] determined the extremal values of the Mostar index among trees and unicyclic graphs, respectively. In 2019, Tepeh [14] characterized the bicyclic graphs with extremal Mostar index.

In the end of [7], the authors stated several conjectures and listed some open problems. One of them is considered the Mostar index among benzenoid chains, catacondensed benzenoids and general benzenoid graphs as follows.

Problem 1.1 ([7]). *Find extremal benzenoid chains, catacondensed benzenoids and general benzenoid graphs with respect to the Mostar index.*

Note that hexagonal chains are the graph representations of an important subclass of benzenoid molecules, namely the so-called unbranched catacondensed benzenoids. In this paper, we characterize the structure of hexagonal chains with the extremal Mostar index, which is a part of Problem 1.1.

A *hexagonal chain* G_n with n hexagons is a graph consisting of n regular hexagons $C_1, C_2, \ldots, C_n$ arranged in sequence, which satisfies the following:

(i) Any two hexagons have at most one common edge,

(ii) For each $1 \leq i < j \leq n$, C_i and C_j have a common edge if and only if $j = i + 1$,

(ii) Each vertex belongs to at most two hexagons.

In recent years, there is a lot of work on hexagonal chains. Gutman [8] studied the extremal hexagonal chains with respect to some topological invariants, including the Hosaya index, the Merrifield-Simmons index and the spectral radius. Zhang [17] determine the ordering of single-corner hexagonal chains with respect to the Merrifield-Simmons index. Zhang and Zhang [18] consider the numbers of k-matchings and k-independent sets of hexagonal chains. Khadikar, et al. [11] calculate the Padmakar-Ivan index of some hexagonal chains. Deng [4] give an algorithm for computing the anti-forcing number of hexagonal chains and determine the bounds of the anti-forcing number of hexagonal chains. For more results on hexagonal chains one may be referred to [3, 5, 6, 15, 16] and the references cited therein.

In this paper, we determine sharp upper and lower bounds of the Mostar index among hexagonal chains with a given number of hexagons, respectively. The extremal hexagonal chains are also characterized. We give some necessary notations and useful lemmas about hexagonal chains in the next section. In Sections 3 and 4, we determine the sharp upper and lower bounds of the Mostar index among hexagonal chains with a given number of hexagons, respectively. The extremal hexagonal chains are also characterized. Thus, we partially solved Problem 1.1.

2. Notations and preliminaries

Let $\mathcal{G}_n$ be the set of all the hexagonal chains with n hexagons. For $G_n \in \mathcal{G}_n$, it is easy to check it has $(4n+2)$ vertices and $(5n+1)$ edges. Furthermore, $d_{G_n}(v) \in \{2,3\}$ for each vertex $v \in V_{G_n}$. For convenience, let $V_3(G_n)$ (or V_3 for short) be the set of all the vertices with degree 3 in a hexagonal chain G_n.

By considering the structure of $G_n[V_3]$, we introduce two significant hexagonal chains. A *linear chain*, denote L_n, is a hexagonal chain with n hexagons satisfying $L_n[V_3] \cong (n-1)K_2$. A *helicene chain*, denote by H_n, is a hexagonal chain with n hexagons satisfying that $H_n[V_3]$ is isomorphic to an $(2n-2)$-order comb, which is a graph obtained by attaching a new pendant vertex to each vertex of P_{n-1}. The hexagonal chains L_n and H_n are depicted in Fig. 1, where $L_n[V_3]$ and $H_n[V_3]$ are indicated by thick edges.

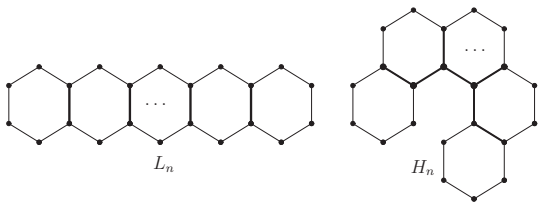


Fig. 1. The linear chain L_n and the helicene chain H_n.

Any hexagonal chain G_n in $\mathcal{G}_n$ can be obtained by connecting two hexagonal chains $B_1 \in \mathcal{G}_{n_1}$ and $B_2 \in \mathcal{G}_{n_2}$ by a single hexagon X, where $n = n_1+n_2+1$. Assume $E_{B_1} \cap E_X = \{ab\}$ and $E_{B_2} \cap E_X = \{xy\}$. If $d_X(a,x) = 1,\ d_X(b,y) = 3$, then we denote $G_n = B_1 \cdot \alpha \cdot B_2$. Similarly, if $d_X(a,x) = d_X(b,y) = 2$ and $d_X(a,x) = 3,\ d_X(b,y) = 1$, then we denote $G_n = B_1 \cdot \beta \cdot B_2$ and $G_n = B_1 \cdot \gamma \cdot B_2$, respectively.(see in Fig. 2.) For convenience, we also use α-type, β-type, γ-type to denote the single hexagon X. In particular, $L_n = L_{n-2} \cdot \beta \cdot C$ and $H_n = H_{n-2} \cdot \alpha \cdot C$, where C is a single hexagon.

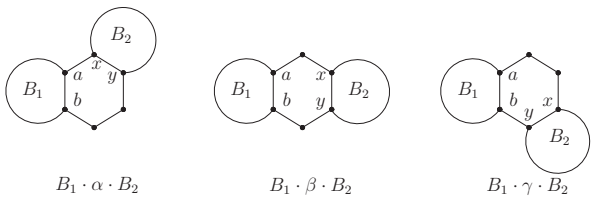


Fig. 2. The three types connecting B_1 and B_2.

Let $G_n \in \mathcal{G}_n$ and $e = uv$ and $f = ab$ be two edges in E_{G_n}. We say e and f are in *parallel relation*, or e is in *parallel relation* with f if and only if $d(u,a) = d(v,b)$ and $d(u,b) = d(v,a)$. Especially, we say each edge is in parallel relation with itself. Denote by $s_{G_n}(e)$ (or $s(e)$ for short) the number of edges in parallel relation with e in G_n. We have the following.

Lemma 2.1. *Let G_n be a hexagonal chain with n hexagons and xy be an edge of G_n. Then,*

(i) *uv is in parallel relation with xy in G_n with $d(u,x) < d(v,x)$ if and only if $x \in N^u_{G_n}(uv),\ y \in N^v_{G_n}(uv)$.*

(ii) *$s(xy) = |\{e = uv \in E_G | x \in N^u_G(e),\ y \in N^v_G(e)\}|$.*

Proof. (i) Firstly, we show the necessity. Since uv is in parallel relation with xy in G_n, one has $d(u,x) = d(v,y),\ d(u,y) = d(v,x)$. Note that $d(u,x) < d(v,x)$. So $x \in N^u_{G_n}(uv)$ and $d(v,y) = d(u,x) < d(v,x) = d(u,y)$, which implies $y \in N^v_{G_n}(uv)$, as desired.

Secondly, we show the sufficiency. Let uv be an edge in E_{G_n} with $x \in N^u_G(uv),\ y \in N^v_G(uv)$, which implies $d(u,x) < d(v,x)$ and $d(u,y) > d(v,y)$. Together with uv and xy are edges of G_n, we get $d(u,x) = d(v,x) - 1$ and $d(v,y) = d(u,y) - 1$. Thus,

$$d(u,x) = d(v,x) - 1 \leq d(v,y) + d(y,x) - 1 = d(v,y) = d(u,y) - 1 < d(u,y),$$

Note that xy is an edge of G_n and recall that $d(u,x) = d(v,x) - 1,\ d(v,y) = d(u,y) - 1$, we get

$$d(u,x) = d(u,y) - 1 = d(v,y), \quad d(u,y) = d(u,x) + 1 = d(v,x).$$

That is, uv is in parallel relation with xy with $d(u,x) < d(v,x)$.

This completes the proof of (i).

(ii) Note that $s(xy)$ is the number of edges in parallel relation with xy in G_n. By (i), (ii) is obvious. ■

Lemma 2.2. *Let $G_n \in \mathcal{G}_n$ and $uv,\ xy$ be two edges in parallel relation in G_n. If $d(u,x) < d(v,x)$, then $N^u_{G_n}(uv) = N^x_{G_n}(xy)$ and $N^v_{G_n}(uv) = N^y_{G_n}(xy)$.*

Proof. One may check that all edges in parallel relation with xy constitute an edge cut, say E_{xy}, of G. Assume $G_x,\ G_y$ are the two components of $G - E_{xy}$ with $x \in V_{G_x}$ and $y \in V_{G_y}$. Clearly, $V_{G_n} = V_{G_x} \cup V_{G_y}$. Note that $d(u,x) < d(v,x)$. For each vertex

$a \in V_{G_x}$, it is easy to check that $d(a,x) < d(a,y)$ and $d(a,u) < d(a,v)$. Similarly, $d(b,x) > d(b,y)$, $d(b,u) > d(b,v)$ for each vertex $b \in V_{G_y}$. Thus,

$$N_G^u(uv) = N_G^x(xy) = V_{G_a},\ N_G^v(uv) = N_G^y(xy) = V_{G_b},$$

which completes the proof. ■

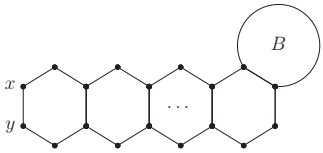


Fig. 3. $L_k \cdot \alpha \cdot B$.

Let $G_n \in \mathcal{G}_n$ and $C_1, C_2, \ldots, C_n$ be the hexagons contained in G_n with $E_{C_i} \cap E_{C_{i+1}} = \{e_i\}$ for $1 \le i \le n-1$. Clearly, there exists an edge $e_0 \neq e_1$ in E_{C_1} such that e_0 is in parallel relation with e_1 in G_n. For convenience, we call e_0 an *end edge* of G_n and have the following.

Lemma 2.3. *Let G_n be a hexagonal chain with n hexagons and $e_0 = xy$ be an end edge of G_n. Then*

(i) *If $G_n \cong L_n$, then $s_{L_n}(xy) = n+1$ and $n_{L_n}^x(xy) = n_{L_n}^y(xy)$.*

(ii) *If $G_n \cong L_k \cdot \alpha \cdot B$, where B is a hexagon chain with $n-k-1(\ge 1)$ hexagons, then $s_{G_n}(xy) = k+2$ and $n_{G_n}^x(xy) - n_{G_n}^y(xy) = 4(n-k-1)$. The graph $L_k \cdot \alpha \cdot B$ is depicted in Fig. 3.*

Proof. (i) By the structure of L_n, it is easy to check $e_1, e_2, \ldots, e_{n-1}$ are in parallel relation with xy in L_n. In addition, there exists an edge $e_n \neq e_{n-1}$ in E_{C_n} such that e_n is in parallel relation with them in L_n. So

$$s_{L_n}(xy) = |\{e_0 = xy, e_1, e_2, \ldots, e_n\}| = n+1.$$

We may assume $e_n = x_n y_n$ with $d(x, x_n) < d(x, y_n)$. Let $P(x, x_n)$ (resp. $P(y, y_n)$) be the shortest path between x and x_n (resp. y and y_n). One may check that $N_{L_n}^x(xy) = |V_{P(x,x_n)}| = 2n+1$, $N_{L_n}^y(xy) = |V_{P(y,y_n)}| = 2n+1$, which implies $n_{L_n}^x(xy) = n_{L_n}^y(xy)$. (i) holds.

(ii) Note that L_k and B are connected by α-type. For each edge $e \in E_B$, it is easy to check that e is not in parallel relation with xy. By a similar proof as (i), we get $s_{G_n}(xy) = k + 2$.

Denote by C the cycle connecting L_k and B in G_n. By the structure of $L_k \cdot \alpha \cdot B$, there exists just two vertices, say a and b, in $V_C \setminus (V_{L_k} \cup V_B)$. One has $N_G^x(xy) = N_{L_k}^x(xy) \cup V_B$ and $N_G^y(xy) = N_{L_k}^y(xy) \cup \{a, b\}$. By (i) we get $n_{L_n}^x(xy) = n_{L_n}^y(xy)$. Thus,

$$n_G^x(xy) - n_G^y(xy) = n_{L_k}^x(xy) + |V_B| - n_{L_k}^y(xy) - 2 = |V_B| - 2 = 4(n - k - 1).$$

This completes the proof of (ii). ■

3. Maximum Mostar index among $\mathcal{G}_n$

In this section, we determine that the helicene chain H_n is the unique graph with maximum Mostar index among $\mathcal{G}_n$. In order to obtain our main result, the following lemma is necessary.

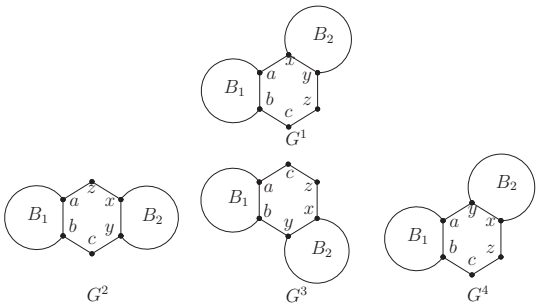


Fig. 4. The graphs G^1, G^2, G^3 and G^4.

Lemma 3.1. *Let $B_1 \in \mathcal{G}_{n_1}$, $B_2 \in \mathcal{G}_{n_2}$ with $n_1 \geq 1$, $n_2 \geq 1$ and $n_1 + n_2 + 1 = n$. Suppose that G^1, G^2, G^3, respectively, are hexagonal chains by connecting B_1 and B_2 by the α-type, β-type and γ-type hexagon X, where $E_{B_1} \cap E_X = \{ab\}$, $E_{B_2} \cap E_X = \{xy\}$. G^4 is a hexagonal chain obtained by reversing the edge xy in G^1. The hexagonal chains G^1, G^2, G^3 and G^4 are depicted in Fig. 4. If $n_{B_1}^a(ab) \geq n_{B_1}^b(ab)$ and $n_{B_2}^x(xy) \geq n_{B_2}^y(xy)$, then*

(i) $Mo(G^1) > Mo(G^2)$.

(ii) $Mo(G^1) \geq Mo(G^3)$ *with equality if and only if* $G^1 \cong G^3$.

(iii) $Mo(G^1) \geq Mo(G^4)$ *with equality if and only if* $G^1 \cong G^4$.

Proof. Clearly, $|V_{B_1}| = 4n_1 + 2$, $|V_{B_2}| = 4n_2 + 2$. Since $n^a_{B_1}(ab) \geq n^b_{B_1}(ab)$, one has $B_1 \cong L_{n_1}$ or may be denoted as $L_{k_1} \cdot \alpha \cdot B$ with $B \in \mathcal{G}_{n_1-k_1-1}$. Furthermore, ab is an end edge of B_1 with $ab \in V_{L_{n_1}}$ or $V_{L_{k_1}}$. By Lemma 2.3, we get $s_{B_1}(ab) = k_1 + 2$ and $n^a_{B_1}(ab) - n^b_{B_1}(ab) = 4(n_1 - k_1 - 1) \geq 0$. (Especially, if $B_1 \cong L_{n_1}$, then denote $n_1 := k_1 + 1$ for convenience. By Lemma 2.3 (i) we also get $s_{B_1}(ab) = n_1 + 1 = k_1 + 2$ and $n^a_{B_1}(ab) - n^b_{B_1}(ab) = 0 = 4(n_1 - k_1 - 1)$). Note that $n^x_{B_2}(xy) \geq n^y_{B_2}(xy)$. Similarly, $B_1 \cong L_{n_2}$ or may be denoted as $L_{k_2} \cdot \alpha \cdot B'$ with $B' \in \mathcal{G}_{n_2-k_2-1}$. Furthermore, xy is an end edge of B_2 with $xy \in V_{L_{n_2}}$ or $V_{L_{k_2}}$. Thus, we also get $s_{B_2}(xy) = k_2 + 2$ and $n^x_{B_2}(xy) - n^y_{B_2}(xy) = 4(n_2 - k_2 - 1) \geq 0$.

(i) By (1.1) we get

$$\begin{aligned} Mo(G^1) - Mo(G^2) &= \sum_{e \in E_{G^1}} \phi_{G^1}(e) - \sum_{e \in E_{G^2}} \phi_{G^2}(e) \\ &= \sum_{e \in E_{B_1}} (\phi_{G^1}(e) - \phi_{G^2}(e)) + \sum_{e \in E_{B_2}} (\phi_{G^1}(e) - \phi_{G^2}(e)) \\ &\quad +(\phi_{G^1}(ax) + \phi_{G^1}(bc) + \phi_{G^1}(cz) + \phi_{G^1}(yz)) \\ &\quad -(\phi_{G^2}(az) + \phi_{G^2}(zx) + \phi_{G^2}(bc) + \phi_{G^2}(cy)). \end{aligned}$$

For convenience, denote $\Lambda_1 = \sum_{e \in E_{B_1}} (\phi_{G^1}(e) - \phi_{G^2}(e))$, $\Lambda_2 = \sum_{e \in E_{B_2}} (\phi_{G^1}(e) - \phi_{G^2}(e))$ and

$$\Lambda_3 = (\phi_{G^1}(ax) + \phi_{G^1}(bc) + \phi_{G^1}(cz) + \phi_{G^1}(yz)) - (\phi_{G^2}(az) + \phi_{G^2}(zx) + \phi_{G^2}(bc) + \phi_{G^2}(cy)).$$

Thus,

$$Mo(G^1) - Mo(G^2) = \Lambda_1 + \Lambda_2 + \Lambda_3. \tag{3.1}$$

Firstly, let us determine Λ_1. Note that B_1 is bipartite. For each edge $e = uv \in E_{B_1}$, we may let $V_{B_1} = N^u_{B_1}(e) \cup N^v_{B_1}(e)$. If a, $b \in N^u_{B_1}(e)$, then

$$N^u_{G^1}(e) = N^u_{G^2}(e) = N^u_{B_1}(e) \cup V_{B_2} \cup \{c, z\}, \quad N^v_{G^1}(e) = N^v_{G^2}(e) = N^v_{B_1}(e),$$

which implies $n^u_{G^1}(e) = n^u_{G^2}(e)$ and $n^v_{G^1}(e) = n^v_{G^2}(e)$. By (1.2), one has

$$\phi_{G^1}(e) - \phi_{G^2}(e) = |n^u_{G^1}(e) - n^v_{G^1}(e)| - |n^u_{G^2}(e) - n^v_{G^2}(e)| = 0.$$

If a, $b \in N^v_{B_1}(e)$, by a similar discussion as above, one can also get $\phi_{G^1}(e) - \phi_{G^2}(e) = 0$. In order to determine Λ_1, it suffices to consider the case $a \in N^u_{B_1}(e)$, $b \in N^v_{B_1}(e)$. By Lemma

2.1 (i), uv is in parallel relation with ab in B_1 and $d(a,u) < d(b,u)$. By Lemma 2.2, we get $N^u_{B^1}(uv) = N^a_{B^1}(ab)$ and $N^v_{B^1}(uv) = N^b_{B^1}(ab)$. Thus,

$$\begin{aligned} N^u_{G^1}(e) &= N^u_{B_1}(uv) \cup V_{B_2} = N^a_{B_1}(ab) \cup V_{B_2}, \\ N^v_{G^1}(e) &= N^v_{B_1}(uv) \cup \{c,z\} = N^b_{B_1}(ab) \cup \{c,z\}. \end{aligned} \tag{3.2}$$

Similarly, we also get xy is in parallel relation with ab in G^2 and then

$$N^u_{G^2}(e) = N^a_{B_1}(ab) \cup N^x_{B_2}(xy) \cup \{z\}, \quad N^v_{G^2}(e) = N^b_{B_1}(ab) \cup N^y_{B_2}(xy) \cup \{c\}. \tag{3.3}$$

Recall that $n^a_{B_1}(ab) - n^b_{B_1}(ab) = 4(n_1 - k_1 - 1) \geq 0$, $n^x_{B_2}(xy) - n^y_{B_2}(xy) = 4(n_2 - k_2 - 1) \geq 0$. Combining (1.2) with (3.2), (3.3), one has

$$\begin{aligned} \phi_{G^1}(e) - \phi_{G^2}(e) &= |n^u_{G^1}(e) - n^v_{G^1}(e)| - |n^u_{G^2}(e) - n^v_{G^2}(e)| \\ &= \left|n^a_{B_1}(ab) + |V_{B_2}| - n^b_{B_1}(ab) - 2\right| \\ &\quad - \left|n^a_{B_1}(ab) + n^x_{B_2}(xy) + 1 - n^b_{B_1}(ab) - n^y_{B_2}(xy) - 1\right| \\ &= \left(n^a_{B_1}(ab) - n^b_{B_1}(ab)\right) + (|V_{B_2}| - 2) \\ &\quad - \left(n^a_{B_1}(ab) - n^b_{B_1}(ab)\right) - \left(n^x_{B_2}(xy) - n^y_{B_2}(xy)\right) \\ &= (|V_{B_2}| - 2) - \left(n^x_{B_2}(xy) - n^y_{B_2}(xy)\right) \\ &= 4n_2 - 4(n_2 - k_2 - 1) \\ &= 4(k_2 + 1). \end{aligned}$$

By Lemma 2.1, $s_{B_1}(ab) = |\{e = uv \in E_{B_1} | a \in N^u_{B_1}(e), b \in N^v_{B_1}(e)\}|$. Hence,

$$\begin{aligned} \Lambda_1 &= \sum_{e=uv \in E_{B_1}} (\phi_{G^1}(e) - \phi_{G^2}(e)) \\ &= \sum_{\substack{e=uv \in E_{B_1} \\ a,b \in N^u_{B_1}(e)}} (\phi_{G^1}(e) - \phi_{G^2}(e)) + \sum_{\substack{e=uv \in E_{B_1} \\ a,b \in N^v_{B_1}(e)}} (\phi_{G^1}(e) - \phi_{G^2}(e)) \\ &\quad + \sum_{\substack{e=uv \in E_{B_1} \\ a \in N^u_{B_1}(e), b \in N^v_{B_1}(e)}} (\phi_{G^1}(e) - \phi_{G^2}(e)) \\ &= 4(k_2+1)|\{e = uv \in E_{B_1} | a \in N^u_{B_1}(e), b \in N^v_{B_1}(e)\}| \\ &= 4(k_2+1)s_{B_1}(ab) \\ &= 4(k_2+1)(k_1+2) > 0. \end{aligned} \tag{3.4}$$

Secondly, by an argument analogous as above, one has

$$\Lambda_2 = \sum_{e \in E_{B_2}} (\phi_{G^1}(e) - \phi_{G^2}(e)) > 0. \tag{3.5}$$

Finally, we consider Λ_3. Without loss of generality, we assume that $n_1 \leq n_2$, which implies $|V_{B_1}| \leq |V_{B_2}|$. It is easy to check that

$$\phi_{G^1}(bc) = \left|n^x_{B_2}(xy) + |V_{B_1}| - n^y_{B_2}(xy) - 2\right|,\ \phi_{G^1}(yz) = \left|n^a_{B_1}(ab) + |V_{B_2}| - n^b_{B_1}(ab) - 2\right|$$

and

$$\phi_{G^1}(ax) = \phi_{G^1}(cz) = \phi_{G^2}(az) = \phi_{G^2}(zx) = \phi_{G^2}(bc) = \phi_{G^2}(cy) = |V_{B_2}| - |V_{B_1}|.$$

Recall that $n^a_{B_1}(ab) - n^b_{B_1}(ab) = 4(n_1 - k_1 - 1) \geq 0,\ n^x_{B_2}(xy) - n^y_{B_2}(xy) = 4(n_2 - k_2 - 1) \geq 0$. Combining (1.2) with (3.2), (3.3), one has

$$\begin{aligned}
\Lambda_3 &= (\phi_{G^1}(ax) + \phi_{G^1}(bc) + \phi_{G^1}(cz) + \phi_{G^1}(yz)) \\
&\quad -(\phi_{G^2}(az) + \phi_{G^2}(zx) + \phi_{G^2}(bc) + \phi_{G^2}(cy)) \\
&= \left|n^x_{B_2}(xy) + |V_{B_1}| - n^y_{B_2}(xy) - 2\right| + \left|n^a_{B_1}(ab) + |V_{B_2}| - n^b_{B_1}(ab) - 2\right| \\
&\quad -2(|V_{B_2}| - |V_{B_1}|) \\
&= (n^x_{B_2}(xy) - n^y_{B_2}(xy)) + (|V_{B_1}| - 2) + (n^a_{B_1}(ab) - n^b_{B_1}(ab)) + (|V_{B_2}| - 2) \\
&\quad -2(|V_{B_2}| - |V_{B_1}|) \\
&= (n^a_{B_1}(ab) - n^b_{B_1}(ab)) + (n^x_{B_2}(xy) - n^y_{B_2}(xy)) + 3|V_{B_1}| - |V_{B_2}| - 4 \\
&= 4(n_1 - k_1 - 1) + 4(n_2 - k_2 - 1) + 3(4n_1 + 2) - (4n_2 + 2) - 4 \\
&= 16n_1 - 4k_1 - 4k_2 - 8. \qquad (3.6)
\end{aligned}$$

Thus, Combining (3.1) with (3.4)-(3.6), one has

$$\begin{aligned}
Mo(G^1) - Mo(G^2) =& \Lambda_1 + \Lambda_2 + \Lambda_3 \\
&> 4(k_2 + 1)(k_1 + 2) + 16n_1 - 4k_1 - 4k_2 - 8 = 16n_1 + 4k_1k_2 + 4k_2 \\
&> 0,
\end{aligned}$$

which implies $Mo(G^1) > Mo(G^2)$, (i) holds.

(ii) By (1.1), similar with the proof of (i) we get

$$Mo(G^1) - Mo(G^3) = \sum_{e \in E_{G^1}} \phi_{G^1}(e) - \sum_{e \in E_{G^3}} \phi_{G^2}(e) = \Lambda_4 + \Lambda_5 + \Lambda_6, \qquad (3.7)$$

where $\Lambda_4 = \sum_{e \in E_{B_1}} (\phi_{G^1}(e) - \phi_{G^3}(e)),\ \Lambda_5 = \sum_{e \in E_{B_2}} (\phi_{G^1}(e) - \phi_{G^3}(e))$ and

$\Lambda_6 = (\phi_{G^1}(ax) + \phi_{G^1}(bc) + \phi_{G^1}(cz) + \phi_{G^1}(yz)) - (\phi_{G^3}(ac) + \phi_{G^3}(by) + \phi_{G^3}(cz) + \phi_{G^3}(zx))$.

Firstly, let us determine Λ_4. For each edge $e = uv \in E_{B_1}$, by an argument analogous to the proof of (i), one has $\phi_{G^1}(e) - \phi_{G^3}(e) = 0$ if a, b are both in $N^u_{B_1}(e)$ or in $N^v_{B_1}(e)$. In order to determine Λ_4, we only need to consider that $a \in N^u_{B_1}(e)$ and $b \in N^v_{B_1}(e)$. In this case, it is easy to check that (3.2) holds and

$$N^u_{G^3}(e) = N^a_{B_1}(e) \cup \{c, z\}, \quad N^v_{G^3}(e) = N^b_{B_1}(e) \cup V_{B_2}. \tag{3.8}$$

Recall that $n^a_{B_1}(ab) - n^b_{B_1}(ab) \geq 0$. Together with (1.2), (3.2) and (3.8), one has

$$\begin{aligned}
\phi_{G^1}(e) - \phi_{G^3}(e) &= |n^u_{G^1}(e) - n^v_{G^1}(e)| - |n^u_{G^3}(e) - n^v_{G^3}(e)| \\
&= \left|n^a_{B_1}(ab) + |V_{B_2}| - n^b_{B_1}(ab) - 2\right| - \left|n^a_{B_1}(ab) + 2 - n^b_{B_1}(ab) - |V_{B_2}|\right| \\
&\geq \left(n^a_{B_1}(ab) - n^b_{B_1}(ab)\right) + (|V_{B_2}| - 2) \\
&\quad - \left(n^a_{B_1}(ab) - n^b_{B_1}(ab)\right) - (|V_{B_2}| - 2) \qquad (3.9) \\
&= 0.
\end{aligned}$$

Note that $n^a_{B_1}(ab) - n^b_{B_1}(ab) \geq 0$ and $|V_{B_2}| - 2 = 4n_2 > 0$. The equation in (3.9) holds if and only if

$$\left|\left(n^a_{B_1}(ab) - n^b_{B_1}(ab)\right) - (|V_{B_2}| - 2)\right| = \left(n^a_{B_1}(ab) - n^b_{B_1}(ab)\right) + (|V_{B_2}| - 2)\,,$$

which implies $n^a_{B_1}(ab) = n^b_{B_1}(ab)$. So $\phi_{G^1}(e) - \phi_{G^3}(e) \geq 0$ with equality if and only if $n^a_{B_1}(ab) = n^b_{B_1}(ab)$.

Hence,

$$\begin{aligned}
\Lambda_4 &= \sum_{e=uv\in E_{B_1}} (\phi_{G^1}(e) - \phi_{G^3}(e)) \\
&= \sum_{\substack{e=uv\in E_{B_1} \\ a,b\in N^u_{B_1}(e)}} (\phi_{G^1}(e) - \phi_{G^3}(e)) + \sum_{\substack{e=uv\in E_{B_1} \\ a,b\in N^v_{B_1}(e)}} (\phi_{G^1}(e) - \phi_{G^3}(e)) \\
&\quad + \sum_{\substack{e=uv\in E_{B_1} \\ a\in N^u_{B_1}(e), b\in N^v_{B_1}(e)}} (\phi_{G^1}(e) - \phi_{G^3}(e)) \\
&\geq 0. \qquad (3.10)
\end{aligned}$$

The equality in (3.10) holds if and only if $n^a_{B_1}(ab) = n^b_{B_1}(ab)$.

Secondly, by an argument analogous as above, one has

$$\Lambda_5 = \sum_{e\in E_{B_2}} (\phi_{G^1}(e) - \phi_{G^3}(e)) \geq 0 \tag{3.11}$$

with equality if and only if $n^x_{B_2}(xy) = n^y_{B_2}(xy)$.

Finally, let us consider Λ_6. It is easy to check that

$$\phi_{G^1}(ax) = \phi_{G^1}(cz) = \phi_{G^3}(by) = \phi_{G^3}(cz) = \left||V_{B_2}| - |V_{B_1}|\right|.$$

Note that $n^x_{B_2}(xy) - n^y_{B_2}(xy) \geq 0$. One has

$$\begin{aligned}
\phi_{G^1}(bc) - \phi_{G^3}(ac) =& \left|n^x_{B_2}(xy) + |V_{B_1}| - n^y_{B_2}(xy) - 2\right| - \left|n^y_{B_2}(xy) + |V_{B_1}| - n^x_{B_2}(xy) - 2\right| \\
=& \left(n^x_{B_2}(xy) - n^y_{B_2}(xy)\right) + (|V_{B_1}| - 2) \\
& - \left|(|V_{B_1}| - 2) - \left(n^x_{B_2}(xy) - n^y_{B_2}(xy)\right)\right| \\
\geq& \left(n^x_{B_2}(xy) - n^y_{B_2}(xy)\right) + (|V_{B_1}| - 2) \\
& - (|V_{B_1}| - 2) - \left(n^x_{B_2}(xy) - n^y_{B_2}(xy)\right) \qquad (3.12) \\
=& 0.
\end{aligned}$$

Similar with (3.9), the equality in (3.12) holds if and only if $n^x_{B_2}(xy) = n^y_{B_2}(xy)$. Note that $n^a_{B_1}(ab) - n^b_{B_1}(ab) \geq 0$, we also get

$$\begin{aligned}
\phi_{G^1}(yz) - \phi_{G^3}(xz) =& \left|n^a_{B_1}(ab) + |V_{B_2}| - n^b_{B_1}(ab) - 2\right| - \left|n^b_{B_1}(ab) + |V_{B_2}| - n^a_{B_1}(ab) - 2\right| \\
=& \left(n^a_{B_1}(ab) - n^b_{B_1}(ab)\right) + (|V_{B_2}| - 2) \\
& - \left|(|V_{B_2}| - 2) - (n^a_{B_1}(ab) - n^b_{B_1}(ab))\right| \\
\geq& \left(n^a_{B_1}(ab) - n^b_{B_1}(ab)\right) + (|V_{B_2}| - 2) \\
& - (|V_{B_2}| - 2) - \left(n^a_{B_1}(ab) - n^b_{B_1}(ab)\right) \qquad (3.13) \\
=& 0.
\end{aligned}$$

The equality in (3.13) holds if and only if $n^a_{B_1}(ab) = n^b_{B_1}(ab)$.

Hence,

$$\begin{aligned}
\Lambda_6 =& (\phi_{G^1}(ax) + \phi_{G^1}(bc) + \phi_{G^1}(cz) + \phi_{G^1}(yz)) \\
& - (\phi_{G^3}(ac) + \phi_{G^3}(by) + \phi_{G^3}(cz) + \phi_{G^3}(zx)) \geq 0 \qquad (3.14)
\end{aligned}$$

with equality if and only if $n^a_{B_1}(ab) = n^b_{B_1}(ab)$ and $n^x_{B_2}(xy) = n^y_{B_2}(xy)$.

Together with (3.7) and (3.10)-(3.14), we get $Mo(G^1) - Mo(G^3) = \Lambda_4 + \Lambda_5 + \Lambda_6 \geq 0$ with equality if and only if $n^a_{B_1}(ab) = n^b_{B_1}(ab)$ and $n^x_{B_2}(xy) = n^y_{B_2}(xy)$. That is, $Mo(G^1) \geq Mo(G^3)$ with equality if and only if $n^a_{B_1}(ab) = n^b_{B_1}(ab)$ and $n^x_{B_2}(xy) = n^y_{B_2}(xy)$. Consider the structure of B_1 and B_2, one has $n^a_{B_1}(ab) = n^b_{B_1}(ab)$ if and only if $B_1 = L_{n_1}$ and ab is

an end edge of B_1; $n^x_{B_2}(xy) = n^y_{B_2}(xy)$ if and only if $B_2 = L_{n_2}$ and xy is an end edge of B_2. Together with the structures of G^1 and G^3, one has $Mo(G^1) \geq Mo(G^3)$ with equality if and only if $G^1 \cong G^3$. This completes the proof of (ii).

(iii) By (1.1), similar with the proof of (i) we get

$$Mo(G^1) - Mo(G^4) = \sum_{e\in E_{G^1}} \phi_{G^1}(e) - \sum_{e\in E_{G^4}} \phi_{G^4}(e) = \Lambda_7 + \Lambda_8 + \Lambda_9$$

where $\Lambda_7 = \sum_{e\in E_{B_1}}(\phi_{G^1}(e) - \phi_{G^4}(e))$, $\Lambda_8 = \sum_{e\in E_{B_2}}(\phi_{G^1}(e) - \phi_{G^4}(e))$ and

$$\Lambda_9 = (\phi_{G^1}(ax) + \phi_{G^1}(bc) + \phi_{G^1}(cz) + \phi_{G^1}(yz)) - (\phi_{G^4}(ay) + \phi_{G^4}(bc) + \phi_{G^4}(cz) + \phi_{G^4}(xz)).$$

Firstly, let us determine Λ_7. For each edge $e = uv \in E_{B_1}$, by an argument analogous to the proof of (i), one has $\phi_{G^1}(e) - \phi_{G^4}(e) = 0$ if a, b are both in $N^u_{B_1}(e)$ or in $N^v_{B_1}(e)$. In order to determine Λ_7, we only need to consider that $a \in N^u_{B_1}(e)$ and $b \in N^v_{B_1}(e)$. Clearly,

$$N^u_{G^1}(e) = N^u_{G^4}(e) = N^u_{B_1}(e) \cup V_{B_2}, \quad N^v_{G^1}(e) = N^v_{G^4}(e) = N^v_{B_1}(e) \cup \{c, z\},$$

which implies $\phi_{G^1}(e) - \phi_{G^4}(e) = 0$. Hence, $\Lambda_7 = \sum_{e=uv\in E_{B_1}}(\phi_{G^1}(e) - \phi_{G^4}(e)) = 0$.

Secondly, let us determine Λ_8. For each edge $e = uv \in E_{B_2}$, by an argument analogous to the proof of (i), one has $\phi_{G^1}(e) - \phi_{G^4}(e) = 0$ if x, y are both in $N^u_{B_2}(e)$ or in $N^v_{B_2}(e)$. In order to determine Λ_8, it suffies to consider the case $x \in N^u_{B_2}(e)$ and $y \in N^v_{B_2}(e)$. In this case, xy and uv are in parallel relation in B_2. Thus,

$$N^u_{G^1}(e) = N^x_{B_2}(xy) \cup V_{B_1}, \quad N^v_{G^1}(e) = N^y_{B_2}(xy) \cup \{c, z\}$$

and

$$N^u_{G^4}(e) = N^x_{B_2}(xy) \cup \{c, z\}, \quad N^v_{G^4}(e) = N^y_{B_2}(xy) \cup V_{B_1}.$$

Thus,

$$\begin{aligned}
\phi_{G^1}(e) - \phi_{G^4}(e) =& \left|n^x_{B_2}(xy) + |V_{B_1}| - n^y_{B_2}(xy) - 2\right| - \left|n^x_{B_2}(xy) + 2 - n^y_{B_2}(xy) - |V_{B_1}|\right| \\
=& \left(n^x_{B_2}(xy) - n^y_{B_2}(xy)\right) + (|V_{B_1}| - 2) \\
& - \left|(n^x_{B_2}(xy) - n^y_{B_2}(xy)) - (|V_{B_1}| - 2)\right| \\
\geq& \left(n^x_{B_2}(xy) - n^y_{B_2}(xy)\right) + (|V_{B_1}| - 2) \\
& - \left(n^x_{B_2}(xy) - n^y_{B_2}(xy)\right) - (|V_{B_1}| - 2) \qquad (3.15) \\
=& 0.
\end{aligned}$$

Similar with (3.9), the equality in (3.15) holds if and only if $n^x_{B_2}(xy) = n^y_{B_2}(xy)$. Hence, $\Lambda_8 = \sum_{e=uv\in E_{B_2}}(\phi_{G^1}(e) - \phi_{G^4}(e)) \geq 0$ with equality if and only if $n^x_{B_2}(xy) = n^y_{B_2}(xy)$.

Finally, let us consider Λ_9. It is easy to check that

$$\phi_{G^1}(ax) = \phi_{G^1}(cz) = \phi_{G^4}(ay) = \phi_{G^4}(cz) = ||V_{B_1}| - |V_{B_2}||.$$

Note that $n^x_{B_2}(xy) \geq n^y_{B_2}(xy)$. By an argument analogous as the determination of Λ_6, one has

$$\begin{aligned}
\Lambda_9 &= (\phi_{G^1}(ax) + \phi_{G^1}(bc) + \phi_{G^1}(cz) + \phi_{G^1}(yz)) \\
&\quad -(\phi_{G^4}(ay) + \phi_{G^4}(bc) + \phi_{G^4}(cz) + \phi_{G^4}(xz)) \\
&= (\phi_{G^1}(bc) - \phi_{G^4}(bc)) + (\phi_{G^1}(yz) - \phi_{G^4}(xz)) \\
&= \left|n^x_{B_2}(xy) + |V_{B_1}| - n^y_{B_2}(xy) - 2\right| - \left|n^y_{B_2}(xy) + |V_{B_1}| - n^x_{B_2}(xy) - 2\right| \\
&\quad + \left|n^a_{B_1}(ab) + |V_{B_2}| - n^b_{B_1}(ab) - 2\right| - \left|n^a_{B_1}(ab) + |V_{B_2}| - n^b_{B_1}(ab) - 2\right| \\
&\geq \left(n^x_{B_2}(xy) - n^y_{B_2}(xy)\right) + (|V_{B_1}| - 2) \\
&\quad - \left(n^x_{B_2}(xy) - n^y_{B_2}(xy)\right) - (|V_{B_1}| - 2) \qquad (3.16) \\
&= 0.
\end{aligned}$$

The equality in (3.16) holds if and only if $n^x_{B_2}(xy) = n^y_{B_2}(xy)$.

Thus, $Mo(G^1) - Mo(G^4) = \Lambda_7 + \Lambda_8 + \Lambda_9 \geq 0$ with equality if and only if $n^x_{B_2}(xy) = n^y_{B_2}(xy)$. That is, $Mo(G^1) \geq Mo(G^4)$ with equality if and only if $n^x_{B_2}(xy) = n^y_{B_2}(xy)$. Consider the structure of B_2, one has $n^x_{B_2}(xy) = n^y_{B_2}(xy)$ if and only if $B_2 = L_{n_2}$ and xy is an end edge of B_2. Together with the structures of G^1 and G^4, one has $Mo(G^1) \geq Mo(G^4)$ with equality if and only if $G^1 \cong G^4$. This completes the proof. ■

Now, let us determine the value of $Mo(H_n)$.

Lemma 3.2. *$Mo(H_n) = 16n^2 - 20n + 6 + 2(-1)^n$, where H_n is a helicene chain with n hexagons, which is depicted in Fig. 1.*

Proof. Note that H_n is a helicene chain with n hexagons, $H_n[V_3]$ is isomorphic to a comb. We may assume $C_1, C_2, \ldots, C_n$ are the n hexagons of H_n with $E_{C_i} \cap E_{C_{i+1}} = \{x_iy_i\}$ and $y_iy_{i+1} \in E_{H_n}$ for $1 \leq i \leq n-1$. Obviously, $\{x_1y_1, x_2y_2, \cdots, x_{n-1}y_{n-1}\} \subset E_{H_n[V_3]}$. For convenience, let $E^1 = \{x_1y_1, x_2y_2, \cdots, x_{n-1}y_{n-1}\}$ and $E^2 = \{y_1y_2, y_2y_3, \cdots, y_{n-2}y_{n-1}\}$. Clearly, $|E^1| = n-1$, $|E^2| = n-2$ and $E_{H_n[V_3]} = E^1 \cup E^2$.

By direct computation, we may obtain $\phi_{H_n}(x_iy_i) = 4n-8$ for $1 \le i \le n-1$ and $\phi_{H_n}(y_iy_{i+1}) = 4(n-2i-1)$ for $i = 1, \ldots, \lfloor \frac{n}{2} \rfloor$. By the symmetry of H_n, we get $\phi_{H_n}(y_iy_{i+1}) = \phi_{H_n}(y_{n-2-i}y_{n-1-i})$ for $i = \lfloor \frac{n}{2} \rfloor + 1, \ldots, n-2$.

For convenience, denote $\widetilde{E^1}$ be the set of edges of H_n who is in parallel relation with one of the edges in E^1. Lemma 2.2 implies that the edges in parallel relation have equal contribution for $Mo(H_n)$. That is, $\phi_{H_n}(e) = 4n-8$ for $e \in \widetilde{E^1}$. Note that there exists just three edges in parallel relation with x_iy_i in H_n for $1 \le i \le n-1$ and $x_iy_i,\ x_jy_j$ are not in parallel relation in H_n for $i \ne j$. One has $\left|\widetilde{E^1}\right| = 3|E^1| = 3(n-1)$. So

$$\sum_{e \in \widetilde{E^1}} \phi_G(e) = 3(n-1)(4n-8) = 12n^2 - 36n + 24.$$

Similarly, denote $\widetilde{E^2}$ be the set of edges of H_n who is in parallel relation with one of the edges in E^2. Note that there exists just two edges in parallel relation with y_iy_{i+1} in H_n for $1 \le i \le n-2$ and $y_iy_{i+1},\ y_jy_{j+1}$ are not in parallel relation in H_n for $i \ne j$. We get $\left|\widetilde{E^2}\right| = 2|E^2| = 2(n-2)$. Furthermore, one has

$$\sum_{e \in \widetilde{E^2}} \phi_G(e) = 2(4(n-3) + 4(n-5) + \cdots + 8 + 0 + 8 + \cdots + 4(n-3)) = 4n^2 - 16n + 12,$$

when n is odd, while

$$\sum_{e \in \widetilde{E^2}} \phi_G(e) = 2(4(n-3) + 4(n-5) + \cdots + 8 + 2 + 8 + \cdots + 4(n-3)) = 4n^2 - 16n + 16,$$

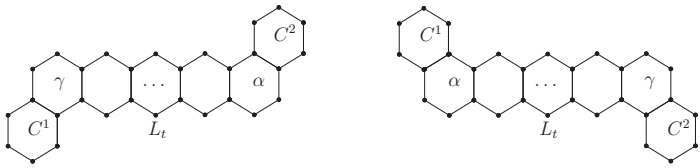
when n is even. That is, $\sum_{e \in \widetilde{E^2}} \phi_G(e) = 4n^2 - 16n + 14 + 2 \cdot (-1)^n$.

Note that H_n is a helicene chain with n hexagons, $E_{H_n} = 5n+1$. Combining with $\left|\widetilde{E^1}\right| = 3(n-1)$ and $\left|\widetilde{E^2}\right| = 2(n-2)$, one has there exists eight edges in $E_{H_n} \setminus (\widetilde{E^1} \cup \widetilde{E^2})$. It is easy to check that $E_{H_n} \setminus (\widetilde{E^1} \cup \widetilde{E^2})$ contains four edges in C_1 and four edges in C_n which are not in parallel relation with x_1y_1 and $x_{n-1}y_{n-1}$, respectively. By direct computation, the contribution of each for $Mo(H_n)$ is $4n-4$.

By (1.1), we have

$$\begin{aligned} Mo(H_n) &= \sum_{e \in \widetilde{E^1}} \phi_G(e) + \sum_{e \in \widetilde{E^2}} \phi_G(e) + \sum_{e \in E_{H_n} \setminus (\widetilde{E^1} \cup \widetilde{E^2})} \phi_G(e) \\ &= 12n^2 - 36n + 24 + 4n^2 - 16n + 14 + 2 \cdot (-1)^n + 8(4n-4) \\ &= 16n^2 - 20n + 6 + 2(-1)^n. \end{aligned}$$

This completes the proof. ■



$C^1 \cdot \gamma \cdot L_t \cdot \alpha \cdot C^2$ $\qquad$ $C^1 \cdot \alpha \cdot L_t \cdot \gamma \cdot C^2$

Fig. 5. $C^1 \cdot \gamma \cdot L_t \cdot \alpha \cdot C^2$ and $C^1 \cdot \alpha \cdot L_t \cdot \gamma \cdot C^2$.

Now, let us give our main result in this section.

Theorem 3.3. *If G_n is a hexagonal chain in $\mathcal{G}_n$, then $Mo(G_n) \leq 16n^2 - 20n + 6 + 2(-1)^n$ with equality if and only if $G_n \cong H_n$.*

Proof. Choose a hexagonal chain G_n in $\mathcal{G}_n$ such that $Mo(G_n)$ is as large as possible. We proceed by showing the following claims.

Claim 1. *If C^1, C^2 are single hexagons and $t \geq 0$, then G_n contains neither $C^1 \cdot \gamma \cdot L_t \cdot \alpha \cdot C^2$ nor $C^1 \cdot \alpha \cdot L_t \cdot \gamma \cdot C^2$ as its subgraph, which are depicted in Fig. 5.*

Proof of Claim 1. By the symmetry, we only need to show G_n does not contain $C^1 \cdot \gamma \cdot L_t \cdot \alpha \cdot C^2$ as its subgraph. Otherwise, suppose that $C^1 \cdot \gamma \cdot L_t \cdot \alpha \cdot C^2$ is a subgraph of G_n satisfying that ab (resp. xy) is the common edge of C^1 and γ (resp. γ and L_t) with $by \in E_{G_n}$. We may denote G_n as $G_p \cdot \theta \cdot C^1 \cdot \gamma \cdot L_t \cdot \alpha \cdot C^2 \cdot \theta \cdot G_q$, where $\theta \in \{\alpha, \beta, \gamma\}$ and $G_p \in \mathcal{G}_p, G_q \in \mathcal{G}_q$ (Maybe $p = 0$ or $q = 0$ and maybe θ does not exist). Let $B_1 = G_p \cdot \theta \cdot C^1$ and $B_2 = L_t \cdot \alpha \cdot C^2 \cdot \theta \cdot G_q$. Thus, $G_n = B_1 \cdot \gamma \cdot B_2$.

Note that $B_2 = L_t \cdot \alpha \cdot C^2 \cdot \theta \cdot G_q$. It is easy to check $n^x_{B_2}(xy) > n^y_{B_2}(xy)$. If $n^a_{B_1}(ab) \geq n^b_{B_1}(ab)$, then by Lemma 3.1 (ii), $B_1 \cdot \alpha \cdot B_2$ is a hexagonal chain in $\mathcal{G}_n$ such that $Mo(B_1 \cdot \alpha \cdot B_2) > Mo(G_n)$, which implies a contradiction with the choice of G_n. Similarly, if $n^a_{B_1}(ab) < n^b_{B_1}(ab)$, then there exists a hexagonal chain G'_n such that $Mo(G'_n) > Mo(G_n)$ by Lemma 3.1 (iii), which is also a contradiction with the choice of G_n.

This completes the proof of Claim 1. ■

Claim 2. *G_n does not contain L_3 as a subgraph.*

Proof of Claim 2. We suppose, to the contrary, $L_3 = C_{q-1}C_qC_{q+1}$ is a subgraph of G_n, where C_i is a single hexagon for $i = q-1, q, q+1$. We may say $L_3 = C_{q-1} \cdot \beta \cdot C_{q+1}$. Similar with Claim 1, we may denote $G_n = B^1 \cdot \beta \cdot B^2$, where C_{q-1} is contained in B^1 and C_{q+1} is contained in B^2, respectively.

Suppose that $a'b'$ (resp. $x'y'$) is the common edges of B^1 and β (resp. B^2 and β). If $n^{a'}_{B^1}(a'b') \geq n^{b'}_{B^1}(a'b')$ and $n^{x'}_{B^2}(x'y') \geq n^{y'}_{B^2}(x'y')$, then by Lemma 3.1 (i), $B^1 \cdot \alpha \cdot B^2$ is a hexagonal chain in $\mathcal{G}_n$ with $Mo(B^1 \cdot \alpha \cdot B^2) > Mo(G_n)$, which implies a contradiction to the choice of G_n. By the symmetry, the remaining case we need to consider is $n^{a'}_{B^1}(a'b') < n^{b'}_{B^1}(a'b')$ and $n^{x'}_{B^2}(x'y') \geq n^{y'}_{B^2}(x'y')$. In this case, one can easily check that G_n contains $C^1 \cdot \gamma \cdot L_t \cdot \alpha \cdot C^2$ as its subgraph, a contradiction with Claim 1.

This completes the proof of Claim 2. ■

Based on Claims 1 and 2, we get $G_n \cong H_n$. Together with Lemma 3.2, our result holds. ■

4. Minimum Mostar index among $\mathcal{G}_n$

In this section, we determine that the linear chain L_n is the unique graph with minimum Mostar index among $\mathcal{G}_n$. In order to do so, the following lemmas are necessary.

Lemma 4.1. *Let $B_1 = L_{n_1},\ B_2 \in \mathcal{G}_{n_2}$ with $n_1 \geq 1,\ n_2 \geq 1,\ n_1 + n_2 + 1 = n$ and ab is an end edge of B_1. Suppose that G^2 and G^3 are hexagonal chains in $\mathcal{G}_n$ by connecting B_1 and B_2 with β-type and γ-type hexagon X, respectively, where $E_{B_1} \cap E_X = \{ab\},\ E_{B_2} \cap E_X = \{xy\}$. Graphs G^2 and G^3 can be seen in Fig. 4. Then $Mo(G^2) \leq Mo(G^3)$ with equality if and only if $B_2 = L_k \cdot \alpha \cdot B$ and $n_1 - n_2 \geq k + 1$, where $B \in \mathcal{G}_{n_2-k-1}$.*

Proof. Clearly, $|V_{B_1}| = 4n_1+2,\ |V_{B_2}| = 4n_2+2$. Note that $B_1 = L_{n_1}$ and ab is an end edge of B_1. By Lemma 2.3(i), one has $s_{B_1}(ab) = n_1 + 1$ and $n^a_{B_1}(ab) = n^b_{B_1}(ab)$. If $n^x_{B_2}(xy) < n^y_{B_2}(xy)$, then by Lemma 3.1 (i) we get $Mo(G^2) < Mo(G^3)$, our result holds. Now, we assume $n^x_{B_2}(xy) \geq n^y_{B_2}(xy)$ in the following. Clearly, B_2 may be denoted as $L_k \cdot \alpha \cdot B$ with $B \in \mathcal{G}_{n_2-k-1}$ and $n_2 \geq k + 1$. Furthermore, xy is an end edge of B_2 with $xy \in E_{L_k}$. By Lemma 2.3 (ii) we get $s_{B_2}(xy) = k + 2$ and $n^x_{B_2}(xy) - n^y_{B_2}(xy) = 4(n_2 - k - 1) \geq 0$. By (1.1) we get

$$Mo(G^2) - Mo(G^3) = \sum_{e \in E_{G^2}} \phi_{G^2}(e) - \sum_{e \in E_{G^3}} \phi_{G^3}(e) = \Gamma_1 + \Gamma_2 + \Gamma_3, \tag{4.1}$$

where $\Gamma_1 = \sum_{e \in E_{B_1}} (\phi_{G^2}(e) - \phi_{G^3}(e)),\ \Gamma_2 = \sum_{e \in E_{B_2}} (\phi_{G^2}(e) - \phi_{G^3}(e))$ and

$\Gamma_3 = (\phi_{G^2}(az) + \phi_{G^2}(zx) + \phi_{G^2}(bc) + \phi_{G^2}(cy)) - (\phi_{G^3}(ac) + \phi_{G^3}(cz) + \phi_{G^3}(zx) + \phi_{G^3}(by))$.

Firstly, let us determine Γ_1. For each edge $e = uv \in E_{B_1}$, by an argument analogous to the proof of Lemma3.1 (i), one has $\phi_{G^2}(e) - \phi_{G^3}(e) = 0$ if a, b are both in $N^u_{B_1}(e)$ or

in $N^v_{B_1}(e)$. So in order to determine Γ_1, we only need to consider that $a \in N^u_{B_1}(e)$ and $b \in N^v_{B_1}(e)$. By Lemma 2.1(i), uv is in parallel relation with ab in B_1 with $d(u,a) < d(v,a)$. By Lemma 2.2, one has $N^u_{B_1}(uv) = N^a_{B_1}(ab)$ and $N^v_{B_1}(uv) = N^b_{B_1}(ab)$. Similarly, we get $N^x_{G^2}(xy) = N^a_{G^2}(ab)$ and $N^y_{G^2}(xy) = N^b_{G^2}(ab)$. Considering the structure of G^2 and G^3, one has

$$N^u_{G^2}(e) = N^a_{B_1}(ab) \cup N^x_{B_2}(xy) \cup \{z\}, \quad N^v_{G^2}(e) = N^b_{B_1}(ab) \cup N^y_{B_2}(xy) \cup \{c\}$$

and

$$N^u_{G^3}(e) = N^a_{B_1}(ab) \cup \{c, z\}, \quad N^v_{G^3}(e) = N^b_{B_1}(ab) \cup V_{B_2}.$$

Recall that $n^a_{B_1}(ab) = n^b_{B_1}(ab)$ and $n^x_{B_2}(xy) - n^y_{B_2}(xy) = 4(n_2 - k - 1) \geq 0$. Together with (1.2), one has

$$\begin{aligned}
\phi_{G^2}(e) - \phi_{G^3}(e) &= |n^u_{G^2}(e) - n^v_{G^2}(e)| - |n^u_{G^3}(e) - n^v_{G^3}(e)| \\
&= \left|n^a_{B_1}(ab) + n^x_{B_2}(xy) + 1 - n^b_{B_1}(ab) - n^y_{B_2}(xy) - 1\right| \\
&\quad - \left|n^a_{B_1}(ab) + 2 - n^b_{B_1}(ab) - |V_{B_2}|\right| \\
&= \left(n^x_{B_2}(xy) - n^y_{B_2}(xy)\right) - (|V_{B_2}| - 2) \\
&= 4(n_2 - k - 1) - 4n_2 \\
&= -4(k+1).
\end{aligned}$$

Since ab is an end edge of B_1, by Lemma 2.1 one has

$$s_{B_1}(ab) = |\{e = uv \in E_{B_1} | a \in N^u_{B_1}(e), b \in N^v_{B_1}(e)\}|.$$

Note that $s_{B_1}(ab) = n_1 + 1$. Thus,

$$\begin{aligned}
\Gamma_1 &= \sum_{e=uv \in E_{B_1}} (\phi_{G^2}(e) - \phi_{G^3}(e)) \\
&= \sum_{\substack{e=uv \in E_{B_1} \\ a,b \in N^u_{B_1}(e)}} (\phi_{G^2}(e) - \phi_{G^3}(e)) + \sum_{\substack{e=uv \in E_{B_1} \\ a,b \in N^v_{B_1}(e)}} (\phi_{G^2}(e) - \phi_{G^3}(e)) \\
&\quad + \sum_{\substack{e=uv \in E_{B_1} \\ a \in N^u_{B_1}(e), b \in N^v_{B_1}(e)}} (\phi_{G^2}(e) - \phi_{G^3}(e)) \\
&= -4(k+1)\left|\{e = uv \in E_{B_1} | a \in N^u_{B_1}(ab), b \in N^v_{B_1}(ab)\}\right| \\
&= -4(k+1)s_{B_1}(ab)
\end{aligned}$$

$$= \quad -4(k+1)(n_1+1). \tag{4.2}$$

Secondly, let us determine Γ_2. For each edge $e = uv \in E_{B_2}$, by an argument analogous to the proof of Lemma 3.1 (i), one has $\phi_{G^2}(e) - \phi_{G^3}(e) = 0$ if $x,\ y$ are both in $N^u_{B_2}(e)$ or in $N^v_{B_2}(e)$. So in order to determine Γ_2, we only need to consider that $x \in N^u_{B_2}(e)$ and $y \in N^v_{B_2}(e)$. By Lemma 2.1 (i), uv is in parallel relation with xy in B_2. By Lemma 2.2, $N^u_{B_2}(uv) = N^x_{B_2}(xy)$ and $N^v_{B_2}(uv) = N^y_{B_2}(xy)$. Thus,

$$N^u_{G^2}(e) = N^a_{B_1}(ab) \cup N^x_{B_2}(xy) \cup \{z\}, \quad N^v_{G^2}(e) = N^v_{B_1}(ab) \cup N^y_{B_2}(xy) \cup \{c\}.$$

and

$$N^u_{G^3}(e) = N^x_{B_2}(xy) \cup \{c, z\}, \quad N^v_{G^3}(e) = N^y_{B_2}(xy) \cup V_{B_1}.$$

Recall that $n^a_{B_1}(ab) = n^b_{B_1}(ab)$ and $n^x_{B_2}(xy) - n^y_{B_2}(xy) = 4(n_2 - k - 1) \geq 0$. Together with (1.2), one has

$$\begin{aligned}
\phi_{G^2}(e) - \phi_{G^3}(e) &= |n^u_{G^2}(e) - n^v_{G^2}(e)| - |n^u_{G^3}(e) - n^v_{G^3}(e)| \\
&= \left|n^a_{B_1}(ab) + n^x_{B_2}(xy) + 1 - n^b_{B_1}(ab) - n^y_{B_2}(xy) - 1\right| \\
&\quad - \left|n^x_{B_2}(xy) + 2 - n^y_{B_2}(xy) - |V_{B_1}|\right| \\
&= \left(n^x_{B_2}(xy) - n^y_{B_2}(xy)\right) - \left|4n_1 - \left(n^x_{B_2}(xy) - n^y_{B_2}(xy)\right)\right| \\
&= 4(n_2 - k - 1) - |4n_1 - 4(n_2 - k - 1)|\,.
\end{aligned}$$

Hence, by an argument analogous as the determination of Γ_1,

$$\begin{aligned}
\Gamma_2 &= \sum_{e=uv\in E_{B_2}} (\phi_{G^2}(e) - \phi_{G^3}(e)) \\
&= \sum_{\substack{e=uv\in E_{B_2} \\ x\in N^u_{B_2}(e), y\in N^v_{B_2}(e)}} 4(n_2 - k - 1) - |4n_1 - 4(n_2 - k - 1)| \\
&= s_{B_2}(xy)\,[4(n_2 - k - 1) - |4n_1 - 4(n_2 - k - 1)|] \\
&= (k+2)\,[4(n_2 - k - 1) - |4n_1 - 4(n_2 - k - 1)|]
\end{aligned} \tag{4.3}$$

Finally, we consider Γ_3. It is easy to check that

$$\begin{aligned}
\phi_{G^2}(az) = \phi_{G^2}(zx) = \phi_{G^2}(cy) = \phi_{G^2}(bc) &= \phi_{G^3}(by) = \phi_{G^3}(cz) \\
&= ||V_{B_1}| - |V_{B_2}|| = 4|n_1 - n_2|, \\
\phi_{G^3}(ac) &= \left||V_{B_1}| + n^y_{B_2}(xy) - n^x_{B_2}(xy) - 2\right|
\end{aligned}$$

$$= \left|n^x_{B_2}(xy) - n^y_{B_2}(xy) - 4n_1\right| = \left|4(n_2 - k - 1) - 4n_1\right|,$$

$$\phi_{G^3}(zx) = \left|n^a_{B_1}(ab) + 2 - n^b_{B_1}(ab) - |V_{B_2}|\right| = |V_{B_2}| - 2 = 4n_2.$$

Thus,

$$\begin{aligned}\Gamma_3 &= (\phi_{G^2}(az) + \phi_{G^2}(zx) + \phi_{G^2}(bc) + \phi_{G^2}(cy)) \\ &\quad -(\phi_{G^3}(ac) + \phi_{G^3}(cz) + \phi_{G^3}(zx) + \phi_{G^3}(by)) \\ &= 8|n_1 - n_2| - 4\left|n_2 - n_1 - k - 1\right| - 4n_2. \end{aligned} \tag{4.4}$$

We proceed by considering the following two cases:

Case 1. $n_1 \geq n_2$. In this case, note that $k \geq 0$, one has $n_1 \geq n_2 > n_2 - k - 1$. By (4.1)-(4.4) one has

$$\begin{aligned} Mo(G^2) - Mo(G^3) &= \Gamma_1 + \Gamma_2 + \Gamma_3 \\ &= -4(k+1)(n_1+1) + 4(k+2)\left[(n_2 - k - 1) - (n_1 - n_2 + k + 1)\right] \\ &\quad +8(n_1 - n_2) + 4(n_2 - n_1 - k - 1) - 4n_2 \\ &= 8(k+1)(n_1 - n_2) - 8k^2 - 32k - 24 \\ &< 0, \end{aligned}$$

which implies $Mo(G^2) < Mo(G^3)$.

Case 2. $n_1 < n_2$. If $n_2 - n_1 < k + 1$, then by (4.1)-(4.4) one has

$$\begin{aligned} Mo(G^2) - Mo(G^3) &= -4(k+1)(n_1+1) + 4(k+2)\left[(n_2 - k - 1) - (n_1 - n_2 + k + 1)\right] \\ &\quad -8(n_1 - n_2) + 4(n_2 - n_1 - k - 1) - 4n_2 \\ &= (8k+24)(n_2 - n_1) - 8k^2 - 32k - 24 \\ &< (8k+24)(k+1) - 8k^2 - 32k - 24 \\ &= 0, \end{aligned}$$

which implies $Mo(G^2) < Mo(G^3)$. Otherwise, $n_2 - n_1 \geq k + 1$. Similarly,

$$\begin{aligned} Mo(G^2) - Mo(G^3) &= -4(k+1)(n_1+1) + 4(k+2)\left[(n_2 - k - 1) + (n_1 - n_2 + k + 1)\right] \\ &\quad -8(n_1 - n_2) - 4(n_2 - n_1 - k - 1) - 4n_2 \\ &= 0. \end{aligned}$$

By Cases 1 and 2, our lemma is obvious. ■

Lemma 4.2. *$Mo(L_n) = 8n^2 - 4 + 4(-1)^n$, where L_n is a linear chain with n hexagons, which is depicted in Fig.1.*

Proof. Suppose that $C_1, C_2, \ldots, C_n$ are the n hexagons of L_n with $E_{C_i} \cap E_{C_{i+1}} = \{x_i y_i\}$ for $1 \leq i \leq n-1$. Let x_0y_0 be an end edge of L_n with $x_0y_0 \in E_{C_1}$. Note that L_n is a linear chain with n hexagons, it is easy to get $x_1y_1,\ x_2y_2,\ \ldots, x_{n-1}y_{n-1}$ are in parallel relation with x_0y_0. Clearly, there exists another edge, say x_ny_n in E_{C_n} with $x_ny_n \neq x_{n-1}y_{n-1}$ and x_ny_n is also in parallel relation with x_0y_0. By Lemma 2.2 and Lemma 2.3 (i), we get $\phi_{L_n}(e_i) = |n_{L_n}^{x_i}(e_i) - n_{L_n}^{y_i}(e_i)| = 0$ for $0 \leq i \leq n$.

Obviously, there exists just four edges other than $x_{i-1}y_{i-1}$ and x_iy_i in E_{C_i} for each $i \in \{1, 2, \ldots, n\}$. Consider the structure of L_n, for each $i \in \{1, 2, \ldots, n\}$, one can easily check that these four edges in E_{C_i} have the common contribution (we denote q_i for convenience) for $Mo(G)$. By direct computation, we obtain

$$q_i = ||V_{L_{i-1}}| - |V_{L_{n-i}}|| = 4|n - 2i + 1|,$$

for $i \in \{1, 2, \ldots, n\}$. Thus, by (1.1) we get

$$\begin{aligned} Mo(L_n) &= 4\sum_{i=1}^{n} q_i = 16\sum_{i=1}^{n} |n - 2i + 1| \\ &= 16\sum_{i=1}^{\lfloor \frac{n}{2} \rfloor}(n - 2i + 1) - 16 \sum_{i=\lfloor \frac{n}{2} \rfloor + 1}^{n} (n - 2i + 1) \\ &= 8n^2 - 4 + 4(-1)^n, \end{aligned}$$

as desired. ■

Theorem 4.3. *If G_n is a hexagonal chain in $\mathcal{G}_n$, then $Mo(G_n) \geq 8n^2 - 4 + 4(-1)^n$ with equality if and only if $G_n \cong L_n$.*

Proof. Choose a hexagonal chain G_n in $\mathcal{G}_n$ such that $Mo(G_n)$ is as small as possible. If $G_n \cong L_n$, then by lemma 4.2, our result holds. Now suppose that $G_n \ncong L_n$ and denote

$$G_n = L_{l_0} \cdot \theta \cdot L_{l_1} \cdot \theta \cdot \cdots \cdot \theta \cdot L_{l_{k-1}} \cdot \theta \cdot L_{l_k},$$

where $l_0 + l_1 + \cdots + l_k = n - k,\ l_i \geq 1$ for $0 \leq i \leq k$ and $\theta \in \{\alpha, \gamma\}$. Without loss of generality, we assume that $l_0 \leq l_k$. Put $B^* := L_{l_1} \cdot \theta \cdot \cdots \cdot \theta \cdot L_{l_{k-1}} \cdot \theta \cdot L_{l_k}$. Obviously, $G_n = L_{l_0} \cdot \theta \cdot B^*$, where $B^* \in \mathcal{G}_{n-l_0-1}$ and

$$l_0 \leq l_k \leq l_1 + \cdots + l_k + k - 1 = n - l_0 - 1.$$

Construct a new graph $\widetilde{G_n} = L_{l_0} \cdot \beta \cdot B^*$. Clearly, $\widetilde{G_n}$ is also in $\mathcal{G}_n$. Note that $G_n = L_{l_0} \cdot \theta \cdot B^*$ with $\theta \in \{\alpha, \gamma\}$. If $\theta = \alpha$, then by Lemma 3.1 (i), $Mo(\widetilde{G_n}) < Mo(G_n)$, which is a contradiction with the choice of G_n. Now we consider that $\theta = \gamma$. Note that $l_0 \leq n - l_0 - 1$. By Lemma 4.1, we get $Mo(\widetilde{G_n}) < Mo(G_n)$, which is also a contradiction with the choice of G_n.

This completes the proof of Theorem 4.3. ■

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